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Uniform approximations for glory scattering and diffraction peaks

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Abstract. Semiclassical approximations are derived for the angular dependence of the scattering cross section $\sigma(\theta)$ for two cases, involving the forward and backward directions, where the classical scattering is infinite. The results are approximations uniform in angle and valid from the ordinary semiclassical region where $\sigma(\theta)$ is $O(\hbar^0)$ right round to $\theta = 0$ or π; for a glory $\sigma(\theta)$ is then $O(\hbar^{-1})$ and the forward diffraction peak $\sigma(\theta)$ is $O(\hbar^{-2})$ or larger, depending on the form of the long-range tail of the scattering potential. The formulae are all expressed in terms of the action functions along the paths of the classical problems.

1. Introduction

This article is about the analytical characterization of certain features in the angular dependence of the cross section for potential scattering. The scattering amplitude $f(\theta)$ only shows finely detailed structure under semiclassical conditions, when many de Broglie wavelengths of the incident particles fit into the scattering region. For most of the angular range a crude semiclassical description (Mott and Massey 1965) is usually adequate: each of the particle paths in the equivalent classical problem (where a parallel beam of particles of energy E and mass m impinges on the scatterer) makes a complex exponential contribution to the scattering, with an *amplitude* of zero order in $\hbar$, proportional to the density of paths in its neighbourhood, and a *phase* equal to the classical action along it, measured in units of $\hbar$. The intensity of scattered radiation—the cross section $\sigma(\theta) = |f(\theta)|^2$—then shows interference oscillations whenever two or more classical paths emerge in the same direction θ; in the extreme classical limit, when $\hbar$ is negligible in comparison with the values of the action function, the oscillations are so fast that no instrument can detect them, and the *average* value of $\sigma(\theta)$ must be taken, which gives the simple classical cross section.

Such a description fails completely near angles where the density of paths, and hence the classical cross section, becomes infinite; the quantum cross section is then large (typically it goes as some inverse power of $\hbar$) but finite, and its angular dependence takes a form which depends on the precise way in which the path density diverges. Because considerable information about the scattering potential $V(r)$ can in principle be obtained from the analysis of experimental cross sections in these anomalous angular regions where $f(\theta)$ is large, it is important to find the best possible mathematical descriptions for the various effects.

In the past *transitional approximations* have been found, which are valid only very near to the critical angles, but fail to merge smoothly with the crude semiclassical path formulae away from these angles (for a list of formulae valid in transition regions, see Felsen 1964). Recently, however, *uniform approximations*, based always on the classical path quantities and valid near to or far from the critical angles, have been found for an increasing number of wave problems (Ludwig 1966, 1967, Berry 1966, Lewis *et al.* 1967—see Berry (1969) for a descriptive review). In potential scattering only the *rainbow effect*, where the divergence arises from a simple caustic in the scattered radiation, and the effects of the *creeping waves* occurring with hard-core potentials have been treated by these methods.

Here we derive uniform approximations for two more scattering phenomena. They both arise from the fact that any paths emerging in the forward ($\theta = 0$) or backward ($\theta = \pi$) directions give rise to a classical cross section which is infinite. The first type of rays of this kind are those which are incident at very large impact parameters; they are only slightly deflected by the tail of the scattering potential and contribute to the *diffraction peak* in and near the forward direction. The classical divergence arises in this case because the number of paths emerging within a small range $d\theta$ about θ increases without limit as θ tends to zero. The second phenomenon arises from rays with *finite* impact parameters which, because of the details of the scattering potential, happen to emerge in the forward or backward direction (perhaps after having wound several times about the origin); such rays, as we shall see, form an *axial caustic*, which demands special treatment. The resulting enhancement of $\sigma(\theta)$ for θ near 0 or π is called the *glory effect* by analogy with the meteorological phenomenon which occurs when light hits water droplets; but this is somewhat of a misnomer, since in the optical case the rays do not reach quite round to the backward direction, and it is necessary to invoke the presence of creeping rays to account for what is observed (Van de Hulst 1957).

2. Transformation of the partial-wave expansion

We start with the exact expansion for the scattering amplitude, namely

$$f(\theta) = -\mathrm{i}\left(\frac{\hbar^2}{2mE}\right)^{1/2} \sum_{l=0}^{\infty} (l+\tfrac{1}{2})\{\exp(2\mathrm{i}\eta_l)-1\}\mathrm{P}_l(\cos\theta) \tag{1}$$

where $\mathrm{P}_l(\cos\theta)$ is the Legendre polynomial and η_l the phase shift for the lth partial wave. The number of non-zero terms in this series is roughly equal to the number of wavelengths fitting into the scattering region, so that (1) is a bad representation under semiclassical conditions. What we do is to transform it into a series of integrals over $\lambda = l+\frac{1}{2}$, using the Poisson sum formula (cf. Berry 1966); this gives

$$f(\theta) = -\mathrm{i}\left(\frac{\hbar^2}{2mE}\right)^{1/2} \sum_{m=-\infty}^{\infty} \exp(-\mathrm{i}m\pi)\int_0^\infty \mathrm{d}\lambda\,\lambda\{\exp(2\mathrm{i}\eta_{\lambda-\frac{1}{2}})-1\}\exp(2\pi\mathrm{i}m\lambda)\mathrm{P}_{\lambda-\frac{1}{2}}(\cos\theta). \tag{2}$$

To investigate the semiclassical aspects of scattering we must approximate $\eta_{\lambda-\frac{1}{2}}$ and $\mathrm{P}_{\lambda-\frac{1}{2}}$ by their asymptotic forms for small $\hbar$; it is more convenient to use as a variable not λ but the angular momentum

$$L = \lambda\hbar. \tag{3}$$

The phase shifts are then given by the JWKB expression

$$\eta_{\lambda-\frac{1}{2}} \equiv \frac{\bar{\eta}(L)}{\hbar}+\mathrm{O}(\hbar)$$
$$= \left(\frac{2mE}{\hbar^2}\right)^{1/2}\left(\int_{r_0}^\infty \left[\left\{1-\frac{V(r)}{E}-\frac{L^2}{2mEr^2}\right\}^{1/2}-1\right]\mathrm{d}r - r_0(L)\right)+\tfrac{1}{2}L\pi+\mathrm{O}(\hbar) \tag{4}$$

where $r_0(L)$ is the outermost zero of the square root (see Mott and Massey 1965).

For the Legendre functions it is not sufficient to use the well-known formula

$$\mathrm{P}_{L/\hbar-\frac{1}{2}}(\cos\theta) \simeq \left(\frac{2\hbar}{\pi L\sin\theta}\right)^{1/2}\left\{\cos\left(\frac{L\theta}{\hbar}-\frac{\pi}{4}\right)+\mathrm{O}(\hbar)\right\} \tag{5}$$

since this is only valid if θ is not within $\hbar/L$ of 0 or π. *Uniformly approximate* formulae which reduce to (6) where it is valid, but are correct (for large $L/\hbar$) right up to the forward or backward directions, were derived by Szegö (1934). The 'forward' formula (valid everywhere except near π) is

$$\mathrm{P}_{L/\hbar-\frac{1}{2}}(\cos\theta) \simeq \left(\frac{\theta}{\sin\theta}\right)^{1/2}\mathrm{J}_0\left(\frac{L\theta}{\hbar}\right) \tag{6}$$

where J_0 is the Bessel function of the first kind, while the 'backward' formula (not valid near $\theta = 0$) is

$$\mathrm{P}_{L/\hbar-\frac{1}{2}}(\cos\theta) \simeq \exp\left(-\frac{\mathrm{i}L\pi}{\hbar}+\frac{\pi}{2}\right)\left(\frac{\pi-\theta}{\sin\theta}\right)^{1/2}\mathrm{J}_0\left\{\frac{L}{\hbar}(\pi-\theta)\right\}. \tag{7}$$

We can insert the results (3), (4), (6) and (7) into (2), and use an integral representation for the Bessel functions. This gives

$$f(\theta) \simeq -\frac{\mathrm{i}}{\hbar(2mE)^{1/2}} \sum_{m=-\infty}^{\infty} \exp(-\mathrm{i}m\pi) I_m \tag{8}$$

where in the 'forward' region

$$I_m = \left(\frac{\theta}{\sin\theta}\right)^{1/2} \frac{1}{\pi} \int_0^{\pi} \mathrm{d}\phi \int_0^{\infty} \mathrm{d}L\, L \left[\exp\left\{\frac{2\mathrm{i}\bar{\eta}(L)}{\hbar}\right\} - \delta_{m0}\right] \exp\left(\frac{2\pi \mathrm{i} m L}{\hbar} - \frac{\mathrm{i}L\theta\cos\phi}{\hbar}\right) \tag{9}$$

and in the 'backward' region

$$I_m = \left(\frac{\pi-\theta}{\sin\theta}\right)^{1/2} \exp\left(\frac{\frac{1}{2}\mathrm{i}\pi}{\pi}\right) \int_0^{\pi} \mathrm{d}\phi \int_0^{\infty} \mathrm{d}L\, L \exp\left\{\frac{2\mathrm{i}\bar{\eta}(L)}{\hbar} + \frac{\mathrm{i}L\pi}{\hbar}(2m-1) - \frac{\mathrm{i}L(\pi-\theta)}{\hbar}\cos\phi\right\}. \tag{10}$$

The δ_{m0} term in (9) indicates that the -1 term which appeared in (1) and (2) has been neglected except in the $m = 0$ 'forward' integral. This is justified, since it would contribute a term of order $\hbar^2$ to each of the I_m while the 'classical' contribution is of order $\hbar$, and we are interested here in this and larger effects; however, the term must be retained in the $m = 0$ 'forward' integral since its contribution there is singular and cancels a similar divergence in the $\exp\{2\mathrm{i}\bar{\eta}(L)/\hbar\}$ term which does not occur for this term in any of the other integrals.

The central problem is now to evaluate the integrals (9) and (10) treating $\hbar$ as a small parameter. We expect to get contributions of order $\hbar^0$ or larger only from those I_m whose exponents have stationary points somewhere on the strip of integration in the (L, ϕ) plane. A *line*, where the exponent is stationary in just one variable—for instance the lines $\phi = 0$ and π, will not give a large enough contribution. The condition for stationary points is obtained by differentiating the exponents with respect to L and ϕ, and is, for the 'forward' integrals,

$$2\frac{\mathrm{d}\bar{\eta}}{\mathrm{d}L} \equiv \Theta(L) = \pm\theta - 2m\pi \tag{11}$$

and for the 'backward' integrals

$$\Theta(L) = \pm(\pi-\theta) - (2m-1)\pi. \tag{12}$$

The function $\Theta(L)$ can be evaluated from (4) and gives the *classical deflection* (positive for net repulsion, negative for attraction) of particles incident with angular momentum L. The ranges of deflection angles contributing to each integral are given in the following table:

Order m of integral	Range of contributing deflections Θ forward	backward
0	π to $-\pi$	2π to 0
1	$-\pi$ to -3π	0 to -2π
2	-3π to -5π	-2π to -4π
3	-5π to -7π	-4π to -6π
etc.	etc.	etc.

The integrals for negative m could only have stationary points for deflections exceeding $+\pi$, which is dynamically impossible; these integrals can therefore be neglected in our semi-classical treatment.

The actual value of the exponent at the ith stationary point where $L = L_i(\theta)$ and $\cos\phi_i = \pm 1$ is in all cases

$$S_i(\theta) \equiv 2\bar{\eta}(L_i(\theta)) - L_i(\theta)\Theta(L_i(\theta)) \tag{13}$$

which is just the *classical action* along the ith path that emerges at the observation angle θ, measured relative to the action along the path of an undeflected particle. An uncritical application of the method of stationary phase to either of the double integrals (9) or (10) then gives, for the 'ray' contribution to $f(\theta)$,

$$f_i(\theta) = -\mathrm{i}\alpha_i\beta_i\gamma_i\left\{\frac{L_i(\theta)}{2mE\sin\theta|\Theta'(L_i(\theta))|}\right\}^{1/2}\exp\left\{\frac{\mathrm{i}S_i(\theta)}{\hbar}\right\} \tag{14}$$

where Θ' denotes $\mathrm{d}\Theta/\mathrm{d}L$, α_i is $\exp(\pm \mathrm{i}\pi/4)$ according as Θ' is positive or negative, β_i is $\exp(\pm \mathrm{i}\pi/4)$ according as the ray i emerges on the same side of the axis as it entered (repulsive) or the opposite side (attractive), and $\gamma_i = \exp(-\mathrm{i}m\pi)$, m being the number of times the ray has crossed the backward direction during its windings about the origin.

The crude semiclassical result (14) diverges for rays emergent in the forward or backward directions, owing to the factor $1/\sin\theta$. If Θ' is finite for the contributing path, then we call this classical divergence the *glory effect*. But for all potentials whose tails extend to infinity there is an additional cause for divergence in that Θ' tends to zero for those distant rays that emerge near the forward direction. Figure 1 shows a classical deflection

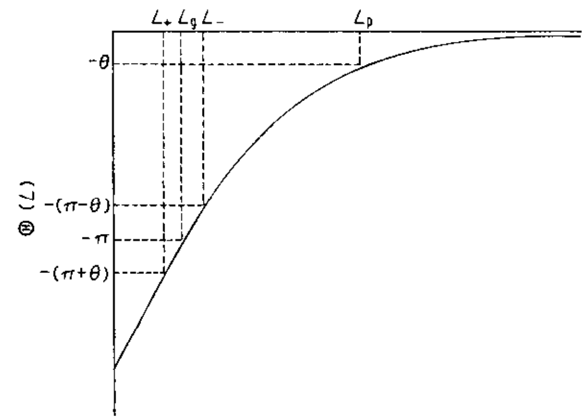

Figure 1.

function, arising from an attractive potential, exhibiting a forward diffraction peak and a backward glory at $\Theta = -\pi$. A forward glory caused by the ray $\Theta = -2n\pi$ involves the $m = n$ integral in (9) while a backward glory caused by $\Theta = -(2n+1)\pi$ involves the $m = n+1$ integral in (10); the diffraction peak is contributed by the large-L tail of the $m = 0$ integral in (9). Simple extrema in $\Theta(L)$, when they do not occur near the forward or backward directions, give rise to rainbow scattering, which has been treated already (Berry 1966).

3. Glory scattering

In mathematical terms it is rather easier to analyse glory scattering, where only the $1/\sin\theta$ factor makes the simple stationary-phase method diverge, than it is to treat the diffraction peak, where Θ' vanishes as well. The analysis is greatly helped by a geometrical picture of the rays and wave fronts for the glory situation. Figure 2 (drawn for a forward glory) shows that the main features are *toroidal wave fronts* and a *caustic* on the axis, which is reached by rays from all azimuth angles (the three-dimensional pattern is generated by rotating figure 2 about the axis). The simplest model of this situation is provided by a *ring source* of radius a, emitting particles of energy E; a short calculation shows that the scattering amplitude is

$$f(\theta) \propto \hbar^{-1/2} J_0 \left\{ \frac{(2mE)^{1/2} a \sin\theta}{\hbar} \right\}$$

$$= \hbar^{-1/2} J_0 \left\{ \frac{S_2(\theta) - S_1(\theta)}{2\hbar} \right\} \tag{16}$$

where S_1 and S_2 are the classical actions (momentum × distance in this case) along the two

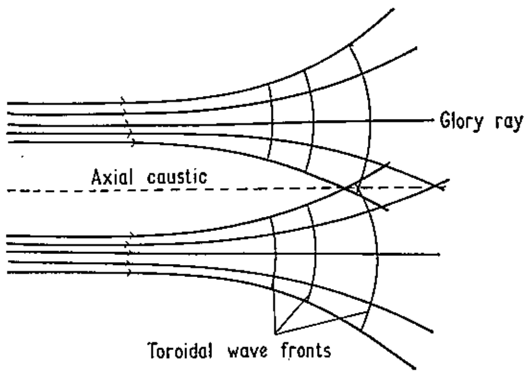

Figure 2.

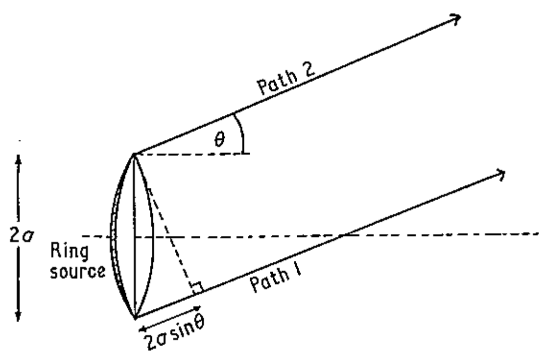

Figure 3.

paths emerging in the direction θ (see figure 3). Under semiclassical conditions $(2mE)^{1/2} a$ is many times greater than $\hbar$, and provided we are not too near the forward direction the argument of the Bessel functions is large enough for the asymptotic form to be used; this is just the crude semiclassical result, where the two rays contribute separately. The essential point is that $\sigma(\theta)$ varies from $O(\hbar^0)$ away from $\theta = 0$ to $O(\hbar^{-1})$ at $\theta = 0$. We shall now derive for our potential scattering problem the appropriate generalization of (16).

Let us label the angular momenta of the two paths contributing at angle θ by $L_{\pm}(\theta)$, where the signs correspond to those in (11) or (12); then as θ approaches 0 or π (depending on whether we are dealing with a forward or a backward glory), $L_+(\theta)$ and $L_-(\theta)$ approach one another and coalesce onto the glory ray L_g (see figure 1). It is quite legitimate to use the simple stationary-phase method for the integral over L; there is just one stationary point, $L(\theta, \phi)$, given by

$$\left. \begin{aligned} \Theta(L) &= -2m\pi + \theta\cos\phi \quad \text{(forward)} \\ \Theta(L) &= -(2m-1)\pi + (\pi - \theta)\cos\phi \quad \text{(backward)} \end{aligned} \right\} \tag{17}$$

and, as ϕ varies over its range from 0 to π, $L(\theta, \phi)$ goes smoothly from $L_+(\theta)$ to $L_-(\theta)$. The result of the evaluation is, for forward glories,

$$I_m \simeq \left(\frac{\theta}{\sin\theta}\right)^{1/2} \frac{\alpha}{\pi}(2\pi\hbar)^{1/2} \int_0^{\pi} \mathrm{d}\phi \frac{L(\theta, \phi)}{|\Theta'(L(\theta, \phi))|^{1/2}} \times \exp\left[\frac{\mathrm{i}}{\hbar}\{2\bar{\eta}L(\theta, \phi) - 2m\pi L(\theta, \phi) - L(\theta, \phi)\theta\cos\phi\}\right] \tag{18}$$

where α is defined following (14). It would be tedious to treat backward glories separately, so we shall just quote the results for this case later. We have ignored the -1 term in I_0 because the glory is a contribution from the neighbourhood of the finite angular-momentum value L_g, and the term in question only acts to make I_0 converge at large L (see § 4).

It is not possible to use the simple stationary-phase method again to evaluate (18), because when θ is nearly zero the exponent is almost constant over the ϕ range, and we do not have the rapidly oscillating integrand essential for the success of the method. But we observe that if it were not for the slow dependence of $L(\theta, \phi)$ on ϕ we would be able to integrate (18) in terms of the zero-order Bessel function. Therefore we apply to this problem an extension of the standard techniques of uniform approximation (see, for example, Chester *et al.* 1957), and change variables in the integral from ϕ to ψ by the mapping

$$2\bar{\eta}(L(\theta, \phi)) - 2\pi m L(\theta, \phi) - L(\theta, \phi)\theta\cos\phi \equiv a(\theta) - b(\theta)\cos\psi. \tag{19}$$

The functions $a(\theta)$ and $b(\theta)$ are determined by the condition that the mapping is one-to-one; thus $\mathrm{d}\psi/\mathrm{d}\phi$ must be finite, and differentiation of (19) with respect to ψ, together with (17), gives

$$\frac{\mathrm{d}\phi}{\mathrm{d}\psi} L(\theta, \phi)\theta\sin\phi = b(\theta)\sin\psi \tag{20}$$

from which we deduce the correspondences

$$\left.\begin{aligned} \phi = 0 &\leftrightarrow \psi = 0 \\ \phi = \pi &\leftrightarrow \psi = \pi \end{aligned}\right\}. \tag{21}$$

If we insert these relations successively into (19), we obtain two equations to be solved for $a(\theta)$ and $b(\theta)$; making use of (13), we obtain the results

$$\left.\begin{aligned} a(\theta) &= \tfrac{1}{2}\{S_+(\theta) + S_-(\theta)\} \equiv \overline{S(\theta)} \\ b(\theta) &= \tfrac{1}{2}\{S_-(\theta) - S_+(\theta)\} \equiv \tfrac{1}{2}\Delta S(\theta) \end{aligned}\right\}. \tag{22}$$

Thus the mean and difference of the actions along the two contributing paths, + and $-$ for the observation angle θ, have appeared naturally. If we change variables in our integral (18) we obtain

$$I_m \simeq \left(\frac{2\pi\hbar\theta}{\sin\theta}\right)^{1/2} \frac{\alpha\exp\{\mathrm{i}\bar{S}(\theta)\}}{\pi} \int_0^{\pi} \mathrm{d}\psi \left\{\frac{L(\theta, \phi(\psi))\,\mathrm{d}\phi(\psi)/\mathrm{d}\psi}{|\Theta(L(\theta, \phi(\psi)))|^{1/2}}\right\} \exp\left\{-\frac{\mathrm{i}\Delta S(\theta)\cos(\psi)}{\hbar}\right\}. \tag{23}$$

To approximate this integral we realize that when θ is not small the integrand oscillates violently and the only contributions come from the stationary points, while when θ is small the factor in curly brackets is almost constant (since $L(\theta, \phi)$ is nearly equal to L_g). If we write

$$\{\} = p(\theta) + q(\theta)\cos\psi + \sin\psi\, h(\psi, \theta) \tag{24}$$

then since the third term is zero at the stationary points we do not expect it to contribute much to the integral, so we neglect it. The resulting expressions are easy to evaluate, and we have

$$I_m \simeq \left(\frac{2\pi\hbar\theta}{\sin\theta}\right)^{1/2} \alpha\exp\left\{\frac{\mathrm{i}\overline{S(\theta)}}{\hbar}\right\}\left[p(\theta)\mathrm{J}_0\left\{\frac{\Delta S(\theta)}{2\hbar}\right\} - \mathrm{i}q(\theta)\mathrm{J}_1\left\{\frac{\Delta S(\theta)}{2\hbar}\right\}\right]. \tag{25}$$

To calculate p and q we put $\psi = 0$ and π successively into (24), to get

$$\left.\begin{aligned} p &= \frac{1}{2}\left\{\frac{L_+(\theta)}{|\Theta'(L_+(\theta))|^{1/2}}\frac{\mathrm{d}\phi(0)}{\mathrm{d}\psi}+\frac{L_-(\theta)}{|\Theta'(L_-(\theta))|^{1/2}}\frac{\mathrm{d}\phi(\pi)}{\mathrm{d}\psi}\right\} \\ q &= \frac{1}{2}\left\{\frac{L_+(\theta)}{|\Theta'(L_+(\theta))|^{1/2}}\frac{\mathrm{d}\phi(0)}{\mathrm{d}\psi}-\frac{L_-(\theta)}{|\Theta'(L_-(\theta))|^{1/2}}\frac{\mathrm{d}\phi(\pi)}{\mathrm{d}\psi}\right\}\end{aligned}\right\}. \tag{26}$$

The derivatives can be calculated by differentiating (20) with respect to ψ and successively putting $\psi = 0$ and $\psi = \pi$, giving

$$\frac{\mathrm{d}\phi(0)}{\mathrm{d}\psi} = \left\{\frac{b(\theta)}{\theta L_+(\theta)}\right\}^{1/2}; \qquad \frac{\mathrm{d}\phi(\pi)}{\mathrm{d}\psi} = \left\{\frac{b(\theta)}{\theta L_-(\theta)}\right\}^{1/2}. \tag{27}$$

If we insert (26) and (27) into (25), we finally obtain for the contribution to the scattering amplitude from a forward glory, whose critical ray emerges with a deflection $-2m\pi$, the result

$$\begin{aligned} f(\theta) = &-\frac{\mathrm{i}\alpha\exp(-\mathrm{i}m\pi)}{2}\left\{\frac{\pi\Delta S(\theta)}{2mE\hbar\sin\theta}\right\}^{1/2}\exp\left\{\frac{\mathrm{i}\overline{S(\theta)}}{\hbar}\right\}\left[\left\{\left(\frac{L_+}{|\Theta_+'|}\right)^{1/2}+\left(\frac{L_-}{|\Theta_-'|}\right)^{1/2}\right\}\mathrm{J}_0\left\{\frac{\Delta S(\theta)}{2\hbar}\right\}\right. \\ &\left.-\mathrm{i}\left\{\left(\frac{L_+}{|\Theta_+'|}\right)^{1/2}-\left(\frac{L_-}{|\Theta_-'|}\right)^{1/2}\right\}\mathrm{J}_1\left\{\frac{\Delta S(\theta)}{2\hbar}\right\}\right]. \end{aligned} \tag{28}$$

If we simply multiply this result by a factor $+\mathrm{i}$ we get the expression for a backward glory whose critical ray emerges with deflection $-(2m-1)\pi$. To check that we really do have a uniform approximation which interpolates correctly between the regions where the cross section is $O(\hbar^0)$ and $O(\hbar^{-1})$ we must evaluate (28) for these two limiting cases.

If we are far enough away from the forward or backward directions for ΔS to be more than several units of $\hbar$, we can replace the Bessel functions by their asymptotic forms; the expression (28) and the similar expression for a backward glory then both reduce to a sum of separate semiclassical contributions from the two contributing rays $+$ and $-$, of the form (14), and a tedious inspection confirms that the factors α, β and γ are correctly given for both types of glory.

Very close to the forward or backward directions we can obtain a transitional approximation to (28). The term involving J_1—which was needed to obtain the correct limiting form far from $\theta = 0$ or π—becomes negligible because L_+ and L_- both approach L_g. To evaluate the first term we use (13) to find $\Delta S(\theta)$ as $\Theta \to \Theta_g$; if S_g is the action along the glory path, we obtain

$$\begin{aligned} S(\Theta) &= 2\bar{\eta}\{L(\Theta)\}-L(\Theta)\Theta \\ &\simeq S_g+(\Theta-\Theta_g)\left\{2\bar{\eta}'(L(\Theta_g))\frac{\mathrm{d}L(\Theta_g)}{\mathrm{d}\Theta}-\frac{\mathrm{d}L(\Theta_g)\Theta_g}{\mathrm{d}\Theta}-L(\Theta_g)\right\} \\ &= S_g-(\Theta-\Theta_g)L_g \end{aligned} \tag{29}$$

so that

$$\begin{aligned} \Delta S(\theta) &= S_- - S_+ = (\Theta_+ - \Theta_-)L_g \\ &= \left.\begin{matrix} 2\theta L_g & \text{(forward)} \\ 2(\pi-\theta)L_g & \text{(backward)}\end{matrix}\right\} \end{aligned} \tag{30}$$

where we have used (11) and (12) for the last line. Thus, very close to the glory, (28) takes the form

$$\begin{aligned} f(\theta) &\simeq -\mathrm{i}\alpha\exp(-\mathrm{i}m\pi)\exp\left(\frac{\mathrm{i}S_g}{\hbar}\right)\left\{\frac{\pi\theta}{mE\hbar\sin\theta|\Theta'(L_g)|}\right\}^{1/2}L_g\mathrm{J}_0\left(\frac{L_g\theta}{\hbar}\right) \qquad \text{(forward)} \\ &\simeq \alpha\exp(-\mathrm{i}m\pi)\exp\left(\frac{\mathrm{i}S_g}{\hbar}\right)\left\{\frac{\pi(\pi-\theta)}{mE\hbar\sin\theta|\Theta'(L_g)|}\right\}^{1/2}L_g\mathrm{J}_0\left\{\frac{L_g(\pi-\theta)}{\hbar}\right\} \qquad \text{(backward).} \end{aligned} \tag{31}$$

Transitional approximations like this were first derived by Ford and Wheeler (1959) in a series of beautiful papers in which they pioneered the application of semiclassical methods to potential scattering, and identified the rainbow and glory effects.

A useful mathematical check on the methods of this section is furnished by their application to the exactly known integral (see Gradshteyn and Ryzhik 1965)

$$I = \frac{1}{\pi}\int_0^\pi \mathrm{d}\phi \int_0^\infty \frac{\mathrm{d}L}{L}\exp\left\{-\frac{\mathrm{i}}{\hbar}\left(L\gamma+\frac{1}{L\delta}+L\theta\cos\phi\right)\right\}$$
$$= -\mathrm{i}\pi \mathrm{H}_0^{(2)}\left\{\frac{(\gamma+\theta)^{1/2}+(\gamma-\theta)^{1/2}}{\hbar\delta^{1/2}}\right\}\mathrm{J}_0\left\{\frac{(\gamma+\theta)^{1/2}-(\gamma-\theta)^{1/2}}{\hbar\delta^{1/2}}\right\} \tag{32}$$

where $\mathrm{H}_0^{(2)}$ is the zero-order Hankel function of the second kind. The exponent has one stationary point if $\theta = 0$, at $L = L_g = (\gamma\delta)^{-1/2}$, and two if $\theta > 0$ given by

$$L_\pm(\theta) = \frac{1}{\{\delta(\gamma\pm\theta)\}^{1/2}}. \tag{33}$$

All the functions appearing in (28) can be evaluated, the term in J_1 vanishes, and the uniform approximation is

$$I \simeq (\pi\hbar)^{1/2}\delta^{1/4}\left\{\frac{(\gamma+\theta)^{1/2}-(\gamma-\theta)^{1/2}}{\theta}\right\}\exp(-\tfrac{1}{4}\mathrm{i}\pi)\exp\left[-\frac{\mathrm{i}}{\hbar\delta^{1/2}}\{(\gamma-\theta)^{1/2}+(\gamma+\theta)^{1/2}\}\right]$$
$$\times \mathrm{J}_0\left\{\frac{(\gamma+\theta)^{1/2}-(\gamma-\theta)^{1/2}}{\hbar\delta^{1/2}}\right\}. \tag{34}$$

But this result, derived by our methods, can also be obtained directly from (32) by replacing $\mathrm{H}_0^{(2)}$ by its asymptotic form. This is justified because the argument of this function is large under semiclassical conditions, when $\hbar$ is much smaller than γ and δ; it would not be justified to use the asymptotic form for J_0 also, since when θ is small enough the argument tends to zero whatever the value of $\hbar$.

4. The diffraction peak in the forward direction

The contribution of the rays of large angular momentum which pass through the long-range tail of the potential and emerge near the forward direction can be calculated from the integral I_0 of (9). It is essential now to retain the term -1 since this makes the integral converge at large L where the integrand no longer oscillates if θ is very small (this does not happen for the other integrals). We can obtain a more convenient form by integrating over L by parts, using the relation

$$\int_0^a x\mathrm{J}_0(x)\,\mathrm{d}x = a\mathrm{J}_1(a). \tag{35}$$

This leads to

$$f(\theta) \simeq \frac{1}{\hbar}\left(\frac{\theta}{2mE\sin\theta}\right)^{1/2}\frac{1}{\mathrm{i}\theta\pi}\int_0^\pi \mathrm{d}\phi\int_0^\infty \mathrm{d}L\, L\Theta(L)\cos\phi\exp\left[\frac{\mathrm{i}}{\hbar}\{2\bar{\eta}(L)-L\theta\cos\phi\}\right] \tag{36}$$

with the factor $\Theta(L)$ now ensuring the convergence instead of the -1 term of (9).

There is now only one stationary point of the exponent, whose angular momentum we shall call $L_p(\theta)$ (see figure 1); the stationary value of $\cos\phi$ is ± 1 depending on whether we are dealing with the + or − case of (11), which in turn depends on whether the long-range potential tail is attractive or repulsive. If θ is not too near zero, it is legitimate to use stationary phase for the integrals over both L and ϕ; this results in a single 'ray' contribution of the form (14). But very near the forward direction $\Theta'(L_p)$ is very small, and (14) diverges. The reason why the stationary-phase method fails is that L_p is so large (see figure 3) that $\bar{\eta}(L)$ is of order $\hbar$ or less, so the exponent in (36) no longer oscillates in the contributing region of L. But in this extreme forward region it obviously suffices to replace $2\bar{\eta}(L)$ by its long-range tail $N(L)$, that is, we assume

$$2\bar{\eta}(L) \underset{L\to\infty}{\to} N(L). \tag{37}$$

We shall then need to evaluate integrals of the form

$$K(\alpha) = -\frac{1}{\mathrm{i}\pi}\int_0^\pi \mathrm{d}\beta \int_0^\infty \mathrm{d}z\, zN'(z)\cos\beta \exp\left[\frac{\mathrm{i}}{\hbar}\{N(z)-z\alpha\cos\beta\}\right] \tag{38}$$

which are simpler than (36) because $N(z)$ is a simpler function than $2\bar{\eta}(L)$.

Unfortunately even for the simplest forms of potential (inverse power, Yukawa, etc.) with corresponding simple forms of tail $N(L)$, the integral $K(\alpha)$ cannot be evaluated in closed form in terms of the known functions of analysis. We shall return to this point later; meanwhile, we show how to get a *uniform approximation* to $f(\theta)$ from (36), which reduces to (38) (with $\alpha = \theta$) for very small angles, but which also gives correctly the ray form for larger angles, even though the phase shift no longer takes on its limiting form (37).

We start by mapping the variables (ϕ, L) of (36) onto (β, z) of (38) by equating the exponents:

$$2\bar{\eta}(L) - L\theta\cos\phi = N(z) - z\alpha\cos\beta \tag{39}$$

where α is an as yet undetermined function of θ. But we need another relation, since we are mapping two variables, so we define z as a function of L alone by using (39) with the angles ϕ and β replaced by their stationary values, i.e.

$$2\bar{\eta}(L) \mp L\theta = N(z) \mp z\alpha \tag{40}$$

where again the upper and lower signs refer to repulsive and attractive deflections. If we imagine solving (40) for $z(L)$ and inserting it into (39) we see that β is a function of both L and ϕ. For the mapping to be one-to-one, the determinant of the transformation must be finite; because z does not depend on ϕ, this factorizes, to give

$$\det\left\|\frac{\partial(L,\phi)}{\partial(z,\beta)}\right\| = \frac{\mathrm{d}L}{\mathrm{d}z}\frac{\partial\phi}{\partial\beta}. \tag{41}$$

To see what this implies, we differentiate (40) with respect to z and (39) with respect to β, which results in

$$\left.\begin{aligned}\{\Theta(L)\mp\theta\}\frac{\mathrm{d}L}{\mathrm{d}z} &= N'(z)\mp\alpha\\ L\theta\sin\phi\frac{\partial\phi}{\partial\beta} &= z\alpha\sin\beta\end{aligned}\right\} \tag{42}$$

so that

$$\det\left\|\frac{\partial(L,\phi)}{\partial(z,\beta)}\right\| = \frac{\sin\beta}{\sin\phi}\,\frac{N'(z)\mp\alpha}{\Theta'(L)\mp\theta}\,\frac{z\alpha}{L\theta}. \tag{43}$$

The first of the three factors in this expression shows that we have to make the indentifications

$$\left.\begin{aligned}\phi = 0 &\leftrightarrow \beta = 0\\ \phi = \pi &\leftrightarrow \beta = \pi\end{aligned}\right\}. \tag{44}$$

The second factor shows that the stationary points in z and L must correspond, i.e. that

$$L = L_{\mathrm{p}}(\theta) \leftrightarrow z = z(\alpha) \tag{45}$$

where

$$N'(z(\alpha)) \mp \alpha = 0. \tag{46}$$

If we insert (45) into (40) we find the following equation which fixes $\alpha(\theta)$:

$$S_p(\theta) = N(z(\alpha)) \mp z(\alpha)\alpha. \tag{47}$$

The final factor $z\alpha/L\theta$ could only diverge or vanish when $\theta \to 0$ and $L \to \infty$; this can be prevented if $\alpha(\theta) \to \theta$ and $z(L) \to L$, which is in fact ensured by the condition (37).

If we substitute the mapping (39) and (40) into (36) we obtain

$$f(\theta) \simeq \frac{1}{\hbar}\left(\frac{\theta}{2mE\sin\theta}\right)^{1/2} \frac{1}{\mathrm{i}\pi\theta}\int_0^{\pi} \mathrm{d}\beta \int_0^{\infty} \mathrm{d}z \left\{\frac{L(z)\Theta(L(z))\cos\phi(z,\beta)}{zN'(z)\cos\beta}\frac{\mathrm{d}L}{\mathrm{d}z}(z)\frac{\mathrm{d}\psi}{\partial\beta}(z,\beta)\right\}$$
$$\times zN'(z)\cos\beta\exp\left[\frac{\mathrm{i}}{\hbar}\{N(z)-z\alpha(\theta)\cos\beta\}\right]. \tag{48}$$

In comparison with the rest of the integrand the first factor in curly brackets is a slowly varying function of z and β; if we replace it by its value at the stationary point ($z = z(\alpha(\theta))$; $\cos\beta = \pm 1$), we shall not be much in error, because for θ not near zero only the neighbourhood of this point contributes to (48) while very near the forward direction the factor is nearly equal to unity. Thus we need to evaluate the derivatives $\mathrm{d}L/\mathrm{d}z$ and $\partial\phi/\partial\beta$ at the stationary point; we do this by differentiating the first of (42) by z and the second by β and setting the variables equal to their stationary values; this gives

$$\frac{\mathrm{d}L}{\mathrm{d}z}(z(\alpha(\theta))) = \left\{\frac{N''(z(\alpha(\theta)))}{\Theta'(L_p(\theta))}\right\}^{1/2}; \qquad \frac{\partial\phi}{\partial\beta}\left(z(\alpha(\theta)), \begin{matrix}0\\ \pi\end{matrix}\right) = \left\{\frac{z(\alpha(\theta))\alpha(\theta)}{L_p(\theta)\theta}\right\}^{1/2}. \tag{49}$$

These results, together with the definition (38), lead, finally, to the following expression for (48) as our uniform approximation for $f(\theta)$:

$$f(\theta) \simeq -\frac{1}{\hbar}\left(\frac{\theta}{2mE\sin\theta}\right)^{1/2}\left\{\frac{N''(z(\alpha(\theta)))}{\Theta'(L_p(\theta))}\frac{\alpha(\theta)}{\theta}\frac{L_p(\theta)}{z(\alpha(\theta))}\right\}^{1/2}\frac{K(\alpha(\theta))}{\alpha(\theta)}. \tag{50}$$

To check that we have a *uniform* approximation, we must evaluate (50) when θ is not near zero; then $\alpha(\theta)$ is large and we can approximate to $K(\alpha)$ by using the method of stationary phase in (38). All quantities relating to the form $N(L)$ of the tail then cancel out, and we are left with a ray contribution of the form (14), with the correct phase factors. In the other limit, $\theta \to 0$, (50) also gives the correct result, since the second square-root factor becomes unity. As an example of how this happens, we shall quote the results of calculations showing how $\alpha(\theta)$ deviates from θ when we take into account small deviations of $2\bar{\eta}(L)$ from its tail when L is large but not infinite; similar expressions show how $z \to L$ and $N'' \to \Theta'$. For an inverse-power phase shift

$$2\bar{\eta}(L) \to \frac{a}{L^n}\left(1+\frac{b}{L}\right) \tag{51}$$

we take the tail $N(L)$ as being the first term, and obtain

$$\alpha(\theta) = \theta\left\{1+\frac{(n+1)b\theta^{1/(n+1)}}{n^2a^{1/(n+1)}(n^{-n/(n+1)}+n^{1/(n+1)})}+\dots\right\}. \tag{52}$$

For an exponential phase shift

$$2\bar{\eta}(L) \to -a\,\mathrm{e}^{-bL}\left(1+\frac{c}{L}\right) \tag{53}$$

the result is

$$\alpha(\theta) = \theta\left[1+\frac{bc}{\{\ln(\theta/ab)\}^2}+\dots\right]. \tag{54}$$

The uniform approximation (50) is the complete formal solution to the problem of the shape of the diffraction peak, but it is useless for practical application unless the comparison functions $K(\alpha)$ are known for the potential tails of common interest. Almost no work has been done on this; the cases of inverse power and exponential potentials have been examined for the forward direction itself by Keller and Levy (1963) and Mason *et al.* (1964) (the latter authors extrapolate their results to non-forward angles by assuming a Gaussian shape for the diffraction peak, but there is no justification for this). The phase-shift tail $N(L)$ is related to the tail of the potential $V(r)$ by the relation

$$N(L) = -\left(\frac{M}{2E}\right)^{1/2} \int_{L/(2mE)^{1/2}}^{\infty} \frac{rV(r)}{(r^2 - L^2/2mE)^{1/2}} \, dr. \tag{55}$$

For a power law potential tail

$$V(r) \to \frac{c}{r^n} \tag{56}$$

the phase-shift tail is

$$N(L) = -\frac{c}{2}\left(\frac{\pi m}{2E}\right)^{1/2} \left(\frac{L^2}{2mE}\right)^{(1-n)/2} \frac{\Gamma\{\frac{1}{2}(n-1)\}}{\Gamma(\frac{1}{2}n)} \equiv -\zeta L^{1-n}. \tag{57}$$

The simplest way of writing the integral which would have to be calculated to find the form of the diffraction peak is

$$S_m(\gamma) \equiv \int_0^{\infty} dx\, x^{-m} J_1(\gamma x) \exp(ix^{-m}) \tag{58}$$

in terms of which

$$K(\alpha) = (n-1)\zeta S_{n-1}\left\{\left(\frac{\zeta}{\hbar}\right)^{1/(n-1)} \frac{\alpha}{\hbar}\right\}. \tag{59}$$

For the forward direction, itself, we find

$$f(0) \simeq -\frac{i\zeta^{2/(n-1)}}{2\hbar^{(n+1)/(n-1)}(2mE)^{1/2}} \Gamma\left(\frac{n-3}{n-1}\right) \exp\left(-\frac{i\pi}{n-1}\right). \tag{60}$$

The simplest exponential-type potential from our point of view is one half-way between a Yukawa and a pure exponential; this has the form

$$V(r) \to \frac{c}{r^{1/2}} e^{-r/a}. \tag{61}$$

The phase-shift tail is

$$N(L) = -\frac{c}{2}\left(\frac{a\pi m}{E}\right)^{1/2} \exp\left\{-\frac{L}{a(2mE)^{1/2}}\right\}. \tag{62}$$

The canonical integral to be evaluated for this case is

$$T(\gamma, \delta) \equiv \int_0^{\infty} dx\, x\, e^{-x} J_1(\delta x) \exp(-i\gamma\, e^{-x}) \tag{63}$$

in terms of which

$$K(\alpha) = amc\left(\frac{\pi a}{2}\right)^{1/2} T\left(\frac{c}{2\hbar}\left(\frac{\pi am}{E}\right)^{1/2}, \frac{a\alpha}{\hbar}(2mE)^{1/2}\right). \tag{64}$$

The forward scattering for this case is

$$f(0) \simeq -\frac{i}{2}\frac{(2mE)^{1/2}a}{\hbar}\left[\ln\left\{\frac{c}{\hbar}\left(\frac{\pi ma}{E}\right)^{1/2}\right\}\right]^2. \tag{65}$$

Classically, the forward scattering from a smooth potential is always infinite, and our results show that the *semi-classical* cross section varies as some increasing function of $1/\hbar$, whose form depends very sensitively on how fast the potential decays at large distances. In all cases, however, $f(0)$ for the diffraction peak is larger than $O(\hbar^{-1})$, whereas for the glory $f(0)$ is $O(\hbar^{-1/2})$. The advantage of the uniform approximation (50) is that it describes correctly the form of the diffraction peak over an angular region where it varies over several orders of magnitude (in a Lennard-Jones potential, for instance, $\sigma(\theta)$ varies from $\hbar^0$ to $\hbar^{-2\cdot 8}$).

5. Conclusion

We have shown that it is possible to set up semiclassical scattering theory in a way which retains contact with the particle paths of the classical problem; the resulting expressions approximate the cross sections uniformly in angle even right into the regions where the classical scattering is infinite. In the case of the glory, our result (28) extends that of Ford and Wheeler (1959) who derived a transitional approximation for the regions very close to $\theta = 0$ or π. Our formula (50) for the diffraction peak involves integrals of the form (38) which are not yet tabulated or fully understood (it would be worth while to make a start by investigating (58) and (63)).

What we have not done is to make our derivations formally complete by deriving higher correction terms to the semiclassical expressions. This would be extremely tedious, and there is no point in undertaking the work until the zero-order terms (which are complicated enough) have been tested numerically or against experiment.

This work, together with studies of the rainbow (Berry 1966, Ludwig 1966) and of the creeping waves occurring with hard-core potentials (Ludwig 1967, Nussenzweig 1965, Rubinow 1961), means that all the common semiclassical potential scattering effects have been treated by methods of uniform approximation with the one exception of orbiting; the pioneer work of Ford and Wheeler (1959) has hardly been improved on, and a uniformly approximate treatment is not yet in sight.

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